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Bixa orellana L. Derived Phytochemicals against Alcohol Dehydrogenase of *Escherichia coli*

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Authors' contributions

This work was carried out in collaboration among all authors. All authors read and approved the final manuscript.

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ABSTRACT

Phytochemicals from *Bixa orellana* L. plant extract are traditionally used to cure Jaundice. It is caused by *Escherichia coli.* Molecular docking method applied using "Biovia Discovery Studio". "High positive values of -CDOCKER energy and -CDOCKER interaction energy" suggested that benzoic acid can effectively deactivate the alcohol dehydrogenase enzyme thereby interrupting the life cycle of the organism.

Keywords: Phytochemical; Bixa orellana L.; Escherichia coli.

1. INTRODUCTION

Nature is a significant wellspring of herbal drugs [1]. The therapeutic estimation of the plants is because of the phytochemicals present in it. Phytochemicals can be gotten from various pieces of plants. Distinctive restorative plants and their phytoextracts have indicated hostile to microbial activity [2]. These restorative plants assume a key job in human medicinal services.

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Numerous individuals depend on the utilization of conventional medication [3].

Bixa orellana belongs to family Bixaceae. *B. orellana* extract is used to cure disease like Jaundice. The objective of the study is to identify the phytochemical responsible to cure the disease.

B. orellana contains “benzoic acid, acetic acid, phenol, anthraquinone” etc. These phytochemicals mightact against *E. coli*. However, there is no such study available.

This objective of the study is to identify the phytochemical of *B. orellana* capable of inhibiting *E. coli* which causes Jaundice.

2. MATERIALS AND METHODS

2.1 Software Used

Discovery studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques to predict the level of molecular interaction.

2.2 Methodology

2.2.1 List of phytochemicals

Phytochemicals are secondary metabolites produced by plants to protect them from predators. The potential threats to plants include bacteria, viruses and fungi. When these plants or their parts are consumed by humans these phytochemicals resist threats to health. Some phytochemicals have been used as poisons and others as traditional medicine. Published works showed that *Bixa orellana* contains norbixin, phytol, phenol, acetic acid, anthraquinone, benzoic acid and farnesyl acetone. It has already been established that *Bixa orellana* plant belonging to Bixaceae family has potential to help controlling Jaundice. This work is focused on identification of specific phytochemical liable for inhibiting and controlling of Jaundice.

2.2.2 Enzyme found in *Escherichia coli*

It has been stated that Jaundice can cause as a result of *Escherichia coli* invasion. In the bacterial life cycle various metabolic cycles have been seen for its existence. These metabolic cycles are controlled by different enzymes. List of different enzymes found in *Escherichia coli* bacteria are detected by using Brenda enzyme database. It has been found that alcohol dehydrogenase enzyme (protein database code 4RQT) is involved in propanol degradation, methionine, Tryptophan, valine, phenylalanine and tyrosine metabolism (BRENDA) and very essential for existence of the specific microbe.

2.2.3 Molecular docking

Molecular docking method has been used to identify the phytochemical from the plant extract that act as a ligand and form a strong covalent bond with the bacterial protein to successfully inhibit the microbe. The Discovery studio module of Biovia software was used for identifying molecular interaction and perform molecular docking. In this process first the sdf files for the phytochemicals found in the *Bixaorellana* plant were downloaded from the website (www.molinstincts.com). The protein database code of the alcohol dehydrogenase enzyme was recognized from the website (www.rcsb.org). The active site of the enzyme was found under "receptor-ligand interaction" and “define and edit binding site” menu via “receptor cavity” protocol. Molecular docking was done under “receptor-ligand interaction” and “Dock ligand” menu by using the CDOCKER protocol of Bioviasoftware. The enzyme act as the receptor molecule and the phytochemical act as the ligand. The quality of molecular docking were indicated by the “-CDOCKER_ENERGY” and “-CDOCKER_INTERACTION_ENERGY”. The high positive value of “-CDOCKER_ENERGY” and “-CDOCKER_INTERACTION_ENERGY” between the ligand and the receptor indicates a good interaction. Thus, the interactions with high values might specify the major phytochemical liable for curing the disease.

3. RESULTS AND DISCUSSION

-CDOCKER energy was calculated based on the internal ligand strain energy and receptor-ligand interaction energy. -CDOCKER interaction signifies the energy of the nonbonded interaction that exists between the protein and the ligand. The criteria for best interaction was chosen based on a) high positive value of -CDOCKER energy and b)small difference between -CDOCKER energy and -CDOCKER interaction energy [4,5]. Table 1 shows that alcohol dehydrogenase-benzoic acid interaction has the highest positive value of -CDOCKER energy (22.2752) and minimum value of the difference (1.0666) between - C DOCKER interaction

Table 1. Results of C docking of phytochemicals with alcohol dehydrogenase (receptor)

Sl. no.	Ligand	-CDOCKER energy	-CDOCKER interaction energy	Difference between -CDOCKER interaction energy and -CDOCKER energy	Remarks
1	Benzoic acid	22.2752	23.3418	1.0666	Maximum inhibition
2	Acetic acid	17.2693	15.3757	1.8936	
3	Phenol	17.2283	19.4368	2.2085	
4	Anthraquinone	22.2749	28.242	5.9671	
5	Phytol	16.0555	46.223	30.1675	
6	Norbixin	1.68869	41.0865	39.39781	
7	Farnesyl acetone	-30.6317	37.9475	68.5792	Minimum inhibition

energy and - C DOCKER energy followed by acetic acid, phenol and anthraquinone. Thus the results indicated that benzoic acid, acetic acid, phenol and anthraquinone can effectively deactivate the alcohol dehydrogenase enzyme thereby interrupting the biological cycle of *Escherichia coli.* Higher positive values for benzoic acid indicated that it was the most active constituent against *Escherichia coli*. On the other hand phytol, norbixin can deactivate the enzyme to a small extent and farnesyl acetone also can deactivate the enzyme to a small extent with negative -CDOCKER energy but positive -CDOCKER interaction energy. Thus, the vital phytochemicals preventing Jaundice caused by *Escherichia coli* are benzoic acid, acetic acid, phenol and anthraquinone.

4. CONCLUSIONS

It was previously known that *Bixaorellana* plant has medicinal action against Jaundice. Jaundice is caused by *Entamoeba histolytica*. This study was carried out to provide the theoretical basis of this observation. Molecular docking operation was executed to identify the phytochemical (benzoic acid, acetic acid, phenol, anthraquinone, phytol, nor-bixin, farnesyl acetone) by using Discovery studio module of Biovia software, which can have a major interaction with the dynamic enzyme (alcohol dehydrogenase) of the microbe. It was found that benzoic acid, acetic acid, phenol and anthraquinone can form a strong bond with the enzyme successfully inhibiting the metabolic cycle of the microbe. Phytol, norbixin and farnesyl acetone were found to be not much effective in deactivating the enzyme of the microbe as they fail to maintain stability. Thus, this study could explain that the presence of benzoic acid, acetic acid, phenol and anthraquinone provided the medicinal values to *Bixaorellana* against Jaundice caused by *Escherichia coli*.

DISCLAIMER

The products used for this research are commonly and predominantly use products in our area of research and country. There is absolutely no conflict of interest between the authors and producers of the products because we do not intend to use these products as an avenue for any litigation but for the advancement of knowledge. Also, the research was not funded by the producing company rather it was funded by personal efforts of the authors.

CONSENT

It is not applicable.

ETHICAL APPROVAL

It is not applicable.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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